Supporting Information: The Interplay of Al and Mg Speciation in Advanced Mg Battery Electrolyte Solutions

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Table S1. Gaussian fit parameters of the XPDF data.

	Peak center (Å)	Area (G(r)·r)	Area (normalized)
0.06 M $MgCl_2$	2.38	0.036	1.0
	3.27	0.069	1.9
	4.07	0.0076	0.21
	4.43	0.038	1.0
	4.82	0.038	1.1
	5.32	0.045	1.3
0.03 M $AlCl_3$	2.19	0.062	1.0
	2.95	0.025	0.41
	3.43	0.020	0.32
	3.78	0.049	0.78
	4.51	0.042	0.68
	4.88	0.035	0.56
	5.34	0.038	0.61
MACC, as-prep.	2.13	0.049	1.0 / 2.0
	2.37	0.025	0.50 / 1.0
	3.25	0.054	1.1 / 2.2
	3.47	0.059	1.2 / 2.4
	4.46	0.070	1.4 / 2.8
	4.88	0.056	1.1 / 2.3
	5.42	0.073	1.5 / 2.9
MACC, cond.	2.15	0.024	1.0 / 0.47
	2.39	0.050	2.1 / 1.0
	3.27	0.079	3.3 / 1.6
	3.49	0.038	1.6 / 0.76
	4.39	0.079	3.3 / 1.6
	4.86	0.068	2.9 / 1.4
	5.35	0.090	3.8 / 1.8

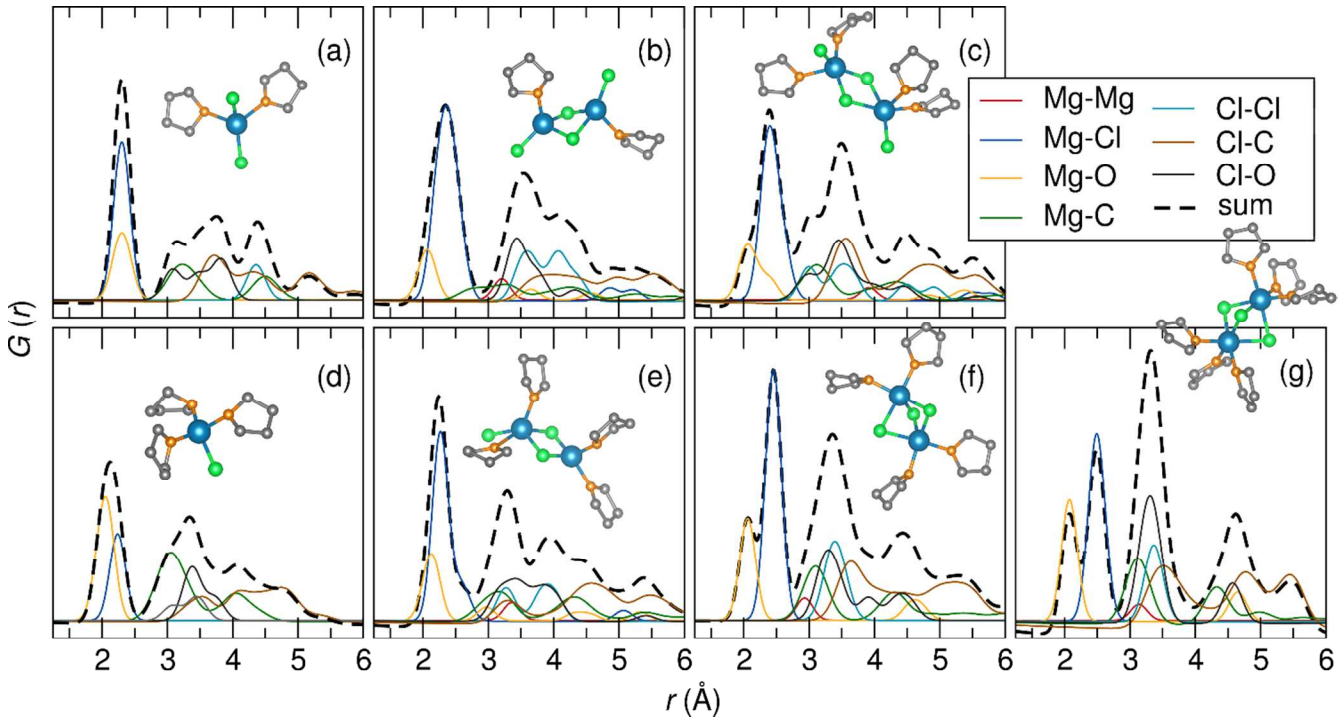

Figure S1. Simulated X-ray PDF patterns of possible Mg complexes in THF. The PDF is simulated with PDFgui using only the complex with the solvent THF removed. (a-c) represent neutral complexes while (d-g) have a nominal charge of +1. The complexes were originally calculated in the (a) liquid, (b) liquid, (c) gas, (d) liquid, (e) liquid, (f) gas, and (g) solid phase.

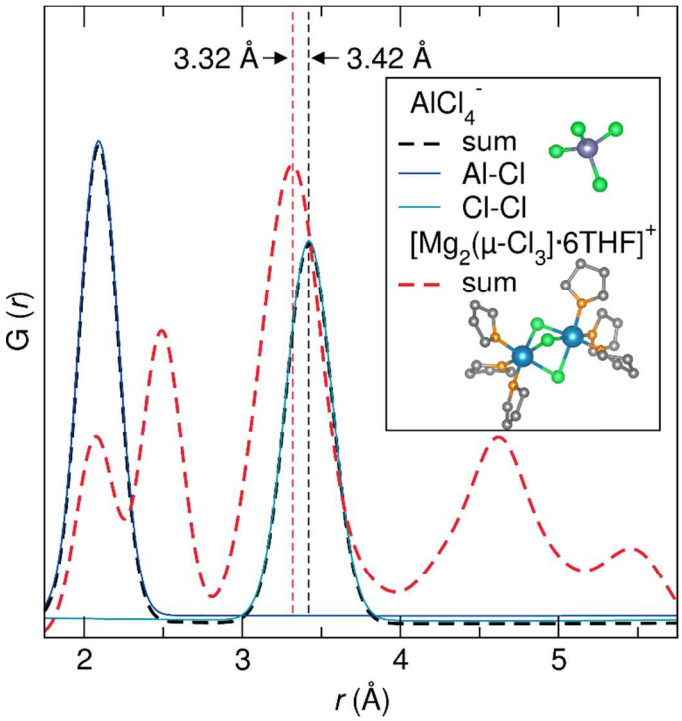

Figure S2. Simulated X-ray PDF patterns of $AlCl_4^-$ and the octahedrally coordinated Mg dimer complex $[Mg_2(\mu\text{–}Cl_3)\cdot THF_6]^+$.

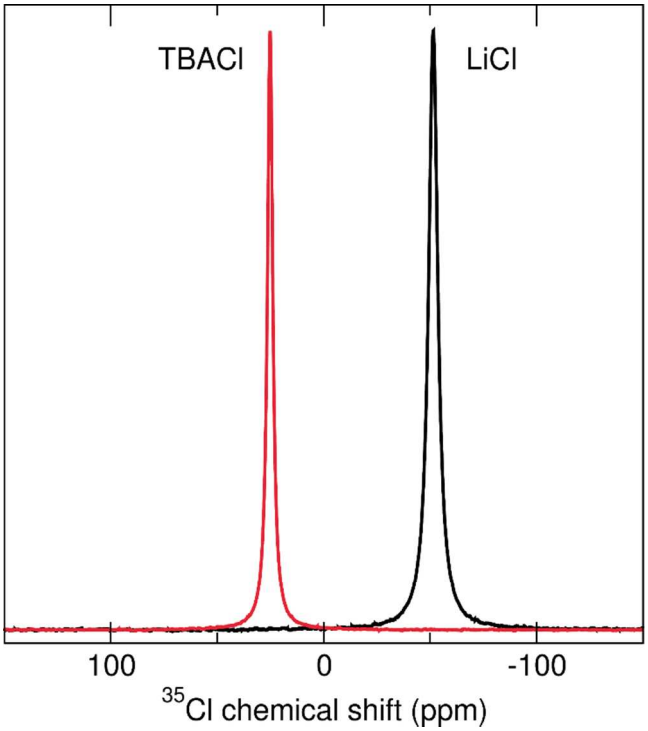

Figure S3. ^{35}Cl NMR of 0.21 M solutions of tetrabutylammonium chloride (TBACl) and lithium chloride (LiCl) in THF. The intensity is normalized.